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Quadrature rule for indefinite integral of algebraic–logarithmic singular integrands

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Abstract

An automatic quadrature method is presented for approximating the indefinite integral of functions having algebraic–logarithmic singularities $Q(x, y, c; f) = \int_x^y f(t)|t-c|^\alpha \log|t-c|\,\mathrm{d}t$, $-1 \leqslant x, y, c \leqslant 1$, $\alpha > -1$, within a finite range $[-1, 1]$ for some smooth function $f(t)$, that is approximated by a finite sum of Chebyshev polynomials. We expand the given indefinite integral in terms of Chebyshev polynomials by using auxiliary algebraic–logarithmic functions. Present scheme approximates the indefinite integral $Q(x, y, c; f)$ uniformly, namely bounds the approximation error independently of the value c as well x and y. This fact enables us to evaluate the integral transform $Q(x, y, c; f)$ with varied values of x, y and c efficiently. Some numerical examples illustrate the performance of the present quadrature scheme.

MSC: 65D30; 65D32; 41A55

Keywords: Quadrature rule; Indefinite integral; Algebraic–logarithmic singularity; Error analysis; Uniform approximation

1. Introduction

Let $f(t)$ be a given smooth function and $K(c; t)$ be a typically badly behaved or singular function such as $\exp(ict)$, $1/(t^2+c^2)$, $|t-c|^\alpha$ and $\log|t-c|$ as well as Cauchy principal value $1/(t-c)$ and Hadamard finite part $1/(t-c)^2$. We consider the evaluation of the product integral

$$\int_{-1}^{1} f(t)K(c; t)\,\mathrm{d}t, \tag{1.1}$$

in particular, the indefinite integral

$$\int_x^y f(t)K(c; t)\,\mathrm{d}t, \quad -1 \leqslant x, y \leqslant 1. \tag{1.2}$$

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There exist rich literature [1,3,7,11,15,17–19] on the numerical evaluation of the definite integral (1.1) for each kernel $K(c;t)$ of the above-mentioned singularities and of some mixed singularities [18,19]. On the other hand, we find little literature on the numerical evaluation of the indefinite integral (1.2) except for our previous papers [8,9], where Hasegawa and Torii construct quadrature formulas of interpolatory type for some types of kernel functions $K(c;t)$, namely $\log|t-c|$, $|t-c|^\alpha$ and $1/(t-c)$, respectively.

In this paper, we propose an automatic quadrature for the indefinite integral of functions involving algebraic–logarithmic singularities

$$Q(x,y,c;f)=\int_x^y f(t)|t-c|^\alpha \log|t-c|\,\mathrm{d}t, \quad \alpha>-1, \tag{1.3}$$

where $-1\leqslant x,y,c\leqslant 1$, within a finite range $[-1,1]$. Specifically, for any fixed triple $\{x_i,y_j,c_l\}$ $(1\leqslant i\leqslant I,\ 1\leqslant j\leqslant J,\ 1\leqslant l\leqslant L)$ we efficiently compute a set of the approximations $\{Q_N(x_i,y_j,c_l)\}$ satisfying

$$|Q(x_i,y_j,c_l;f)-Q_N(x_i,y_j,c_l;f)|\leqslant \max(\varepsilon_a,\varepsilon_r|Q(x_i,y_j,c_l)|), \tag{1.4}$$

for the required absolute (relative) tolerance ε_a (ε_r). The computation of integrals of algebraic–logarithmic singular integrands is required to solve some integral equations derived from the Schrödinger equation in nuclear physics [14].

The present scheme is an extension of the Clenshaw and Curtis method (henceforth abbreviated to CC method) to the integral (1.3). In the CC method, the function $f(t)$ is interpolated by a sum of the Chebyshev polynomials $T_k(t)$ of the first kind:

$$p_N(t)=\sum_{k=0}^{N}{}'' a_k^N T_k(t), \quad -1\leqslant t\leqslant 1. \tag{1.5}$$

The double prime denotes the summation where the first and last terms are halved. The sample points t_j used to interpolate $f(t)$ are $t_j=\cos(\pi j/N)$, $0\leqslant j\leqslant N$, that are zeros of the polynomial $\omega_{N+1}(t)$ defined by

$$\omega_{N+1}(t)=T_{N+1}(t)-T_{N-1}(t)=2(t^2-1)U_{N-1}(t), \tag{1.6}$$

where $U_k(t)$ is the Chebyshev polynomial of the second kind defined by $U_{k-1}(t)=\sin k\theta/\sin\theta$, $t=\cos\theta$. The interpolation condition $f(\cos\pi j/N)=p_N(\cos\pi j/N)$, $0\leqslant j\leqslant N$, determines the coefficients a_k^N of $p_N(t)$ (1.5) as follows:

$$a_k^N=\frac{2}{N}\sum_{j=0}^{N}{}'' f(\cos\pi j/N)\cos(\pi kj/N), \quad 0\leqslant k\leqslant N. \tag{1.7}$$

It is known that the right-hand side of (1.7) can be efficiently computed by means of the fast Fourier transform (FFT) [6,13]. If $f(t)$ is a smooth function, the sum of the Chebyshev polynomials (1.5) converges rapidly as N goes towards infinity.

In their adaptive quadrature programs [20], Piessens et al. use the approximation $p_N(t)$ (1.5) to evaluate the definite integral (1.1)

$$\int_{-1}^{1} f(t)K(c;t)\,\mathrm{d}t \approx \sum_{k=0}^{N} a_k^N M_k, \tag{1.8}$$

where the modified moment M_k is given by $M_k=\int_{-1}^{1}T_k(t)K(c;t)\,\mathrm{d}t$, which can be evaluated for some useful kernel functions by means of recurrence relations [18]. If $K(c;t)=1$, then the quadrature scheme in (1.8) reduces to the CC method.

In this paper, to construct an automatic quadrature scheme of nonadaptive type for the indefinite integral (1.3), we modify the (1.8) to obtain the approximation $Q_N(x,y,c;f)$:

$$Q_N(x,y,c;f)=Q(x,y,c;p_N)=\int_x^y p_N(t)|t-c|^\alpha\log|t-c|\,\mathrm{d}t. \tag{1.9}$$

In Section 2 we demonstrate that it is easy to evaluate $Q(x, y, c; p_N)$ (1.9) (see Lemma 2.1 below). In fact, let $F_N(t)$ and $G_N(t)$ be functions satisfying the following relation:

$$\begin{aligned}&\int \{p_N(t) - p_N(c)\}|t-c|^\alpha \log|t-c|\,\mathrm{d}t\\&\quad = [\{F_N(t) - F_N(c)\}\log|t-c| + G_N(t) - G_N(c)](t-c)|t-c|^\alpha.\end{aligned} \tag{1.10}$$

Then $F_N(t)$ and $G_N(t)$ prove to be polynomials of degree N, respectively. Let $F_N(t)$ and $G_N(t)$ be expressed in terms of the Chebyshev polynomials, then their coefficients can be evaluated by using two three-term recurrence relations. See Section 2 for details.

Section 3 discusses the convergence result and error estimate. Our quadrature formula gives the uniform approximation, namely the approximation error is bounded independently of the values of x, y and $c \in [-1, 1]$. In our previous paper [8,9] we proposed uniform approximation methods for indefinite integrals with $K(c; t) = \log|t-c|$ and $K(c; t) = |t-c|^\alpha$, while for Cauchy kernel $K(c; t) = 1/(t-c)$ the uniform approximation to the indefinite integral remains an open problem. In Section 4 we demonstrate the performance of the present quadrature scheme by using some numerical examples. In Section 5, we prove a theorem used in Section 3.

2. Evaluating the approximation to the indefinite integral

We begin by deriving the expressions of $F_N(t)$ and $G_N(t)$ in (1.10) in terms of the Chebyshev polynomials. Differentiating both sides of (1.10) with respect to t yields

$$\begin{aligned}&\{p_N(t) - p_N(c)\}|t-c|^\alpha \log|t-c|\\&\quad = [(t-c)G_N'(t) + (\alpha+1)\{G_N(t) - G_N(c)\} + F_N(t) - F_N(c)\\&\qquad + [(t-c)F_N'(t) + (\alpha+1)\{F_N(t) - F_N(c)\}]\log|t-c|]|t-c|^\alpha.\end{aligned} \tag{2.1}$$

The solutions of the following differential equations:

$$(t-c)F_N'(t) + (\alpha+1)\{F_N(t) - F_N(c)\} = p_N(t) - p_N(c), \tag{2.2}$$

$$(t-c)G_N'(t) + (\alpha+1)\{G_N(t) - G_N(c)\} + F_N(t) - F_N(c) = 0, \tag{2.3}$$

give $F_N(t)$ and $G_N(t)$ satisfying Eq. (2.1). It can be seen from (2.2) and (2.3) that $F_N(t)$ and $G_N(t)$ are polynomials of degree N, respectively, because $p_N(y)$ is a polynomial of degree N. Therefore, we can write $F_N'(t)$ and $G_N'(t)$ in the forms:

$$F_N'(t) = {\sum_{k=0}^{N-1}}' b_k T_k(t), \quad G_N'(t) = {\sum_{k=0}^{N-1}}' d_k T_k(t), \tag{2.4}$$

respectively, where the prime denotes the summation whose first term is halved.

Integrating both sides of the first equation in (2.4) gives

$$F_N(t) - F_N(c) = \sum_{k=1}^{N} \frac{b_{k-1} - b_{k+1}}{2k}\{T_k(t) - T_k(c)\}, \tag{2.5}$$

where we assume that $b_N = b_{N+1} = 0$. Now, we define that $b_{-1} = b_1$. Since

$$(t-c)F_N'(t) = \frac{1}{2}{\sum_{k=0}^{N}}'(b_{k+1} - 2cb_k + b_{k-1})T_k(t),$$

we have from (1.5), (2.2) and (2.5) the recurrence relation satisfied by b_k

$$(k-\alpha-1)b_{k+1} - 2ckb_k + (k+\alpha+1)b_{k-1} = 2ka_k^N, \quad k \geqslant 1, \tag{2.6}$$

where we use $a_N^N/2$ instead of a_N^N. The coefficients b_k in (2.4) can be stably computed by using the recurrence relation (2.6) in the backward direction with starting values $b_N = b_{N+1} = 0$.

Similarly, we have from (2.3) and (2.4) the recurrence relation satisfied by d_k

$$(k-\alpha-1)d_{k+1} - 2ckd_k + (k+\alpha+1)d_{k-1} = b_{k+1} - b_{k-1}, \quad k \geqslant 1, \tag{2.7}$$

and can stably compute d_k by using (2.7) in the backward direction with starting values $d_N = d_{N+1} = 0$ and with b_k $(0 \leqslant k < N)$ obtained by (2.6).

We establish Lemma 2.1 below by using (1.9) and (1.10) and the relation

$$\int |t-c|^\alpha \log|t-c|\,\mathrm{d}t = \frac{(t-c)|t-c|^\alpha}{\alpha+1}\left\{\log|t-c| - \frac{1}{\alpha+1}\right\}. \tag{2.8}$$

Lemma 2.1. *Let $\Phi_N(t)$ and $\Psi_N(t)$ be defined by*

$$\Phi_N(t) = F_N(t) - F_N(c) + \frac{p_N(c)}{\alpha+1}, \quad \Psi_N(t) = G_N(t) - G_N(c) - \frac{p_N(c)}{(\alpha+1)^2},$$

respectively. Then we have the approximation $Q_N(x, y, c; f)$, $-1 \leqslant x, y, c \leqslant 1$, to the indefinite integral $Q(x, y, c; f)$ given by (1.3),

$$\begin{aligned} Q_N(x, y, c; f) &= (y-c)|y-c|^\alpha\{\Phi_N(y)\log|y-c| + \Psi_N(y)\} \\ &\quad - (x-c)|x-c|^\alpha\{\Phi_N(x)\log|x-c| + \Psi_N(x)\}. \end{aligned}$$

3. Convergence result and error estimate

We begin with the convergence result of our interpolatory integration rules followed by their error estimates. We use the notation

$$\|f\|_p = \left\{\int_{-1}^{1} |f(t)|^p\,\mathrm{d}t\right\}^{1/p}, \quad 1 \leqslant p < \infty,$$

while $\|f\|_\infty = \operatorname{ess\,sup}_{-1\leqslant t\leqslant 1}|f(t)|$.

Lemma 3.1. *Let $f(t)$ be a continuous function on* $[-1, 1]$. *Let $p_N(t)$ be a polynomial interpolating $f(t)$ at the zeros of $\omega_{N+1}(t)$ defined by* (1.6). *Then the quadrature rule $Q_N(x, y, c; f)$ defined by* (1.9) *converges uniformly to the integral $Q(x, y, c; f)$ as $N \to \infty$.*

Proof. Let $K_{\alpha,c}(t) = |t-c|^\alpha \log|t-c|$ and $e_N(t) = f(t) - p_N(t)$. Let $1 \leqslant p \leqslant \infty$ and $1 \leqslant q \leqslant \infty$ such that $1/p + 1/q = 1$. We note that

$$\begin{aligned} |Q(x, y, c; f) - Q_N(x, y, c; f)| &= |Q(x, y, c; f - p_N)| \\ &= \left|\int_x^y K_{\alpha,c}(t)e_N(t)\,\mathrm{d}t\right| \\ &\leqslant \left|\int_{-1}^{1} K_{\alpha,c}(t)e_N(t)\,\mathrm{d}t\right| \leqslant \|K_{\alpha,c}\|_p\|e_N\|_q, \end{aligned} \tag{3.1}$$

where the last relation of (3.1) is Hölder's inequality [21, p. 17]. Since by using [16, Theorem 3.1] we can show that $\|e_N\|_q \to 0$ as $N \to \infty$ for $1 \leqslant q < \infty$, it suffices to show that $\|K_{\alpha,c}\|_p < \infty$ for $-1 < \alpha$. We choose $p = \alpha + 2$ and $q = (\alpha+2)/(\alpha+1)$, then we have $-1 < \alpha p$ since $-1 < \alpha$. It is easy to verify that $\|K_{\alpha,c}\|_p < \infty$. $\square$

Next we estimate the error of the quadrature rule (1.9). Let $\mathscr{E}_\rho$ be an ellipse in the complex plane $z = x + \mathrm{i}y$ with foci $(-1, 0)$, $(1, 0)$ and the semimajor axis $(\rho + \rho^{-1})/2$ and the semiminor axis $(\rho - \rho^{-1})/2$ for a constant $\rho > 1$.

Lemma 3.2. *Assume that $f(z)$ is single valued and analytic inside and on $\mathscr{E}_\rho$. Define $V_k^N(f)$ by a contour integral as follows*:

$$V_k^N(f) = (\pi^2 \mathrm{i})^{-1} \oint_{\mathscr{E}_\rho} \widetilde{U}_k(z) f(z)/\omega_{N+1}(z)\,\mathrm{d}z, \quad k \geqslant 0. \tag{3.2}$$

The Chebyshev function of the second kind $\widetilde{U}_k(z)$ in (3.2) is defined by

$$\widetilde{U}_k(z) = \int_{-1}^{1} \frac{T_k(t)\,\mathrm{d}t}{(z-t)\sqrt{1-t^2}} = \frac{\pi}{\sqrt{z^2-1}w^k} = \frac{2\pi}{(w-w^{-1})w^k}, \tag{3.3}$$

where $w = z + \sqrt{z^2-1}$ and $|w| > 1$ for $z \notin [-1, 1]$. Then, the error for the approximation $Q_N(x, y, c; f)$ (1.9) is given by

$$Q(x, y, c; f) - Q_N(x, y, c; f) = {\sum_{k=0}^{\infty}}' V_k^N(f)\Omega_k^N(x, y, c), \tag{3.4}$$

for $-1 \leqslant x, y, c \leqslant 1$, where $\Omega_k^N(x, y, c)$ is defined by

$$\Omega_k^N(x, y, c) = \int_x^y \omega_{N+1}(t) T_k(t) |t-c|^\alpha \log|t-c|\,\mathrm{d}t, \quad \alpha > -1. \tag{3.5}$$

Proof. The error $f(t) - p_N(t)$ of $p_N(t)$ given by (1.5) can be expressed in terms of a contour integral [4,5,10], which is also expanded in a Chebyshev series [12]:

$$f(t) - p_N(t) = \frac{1}{2\pi \mathrm{i}} \oint_{\mathscr{E}_\rho} \frac{\omega_{N+1}(t) f(z)\,\mathrm{d}z}{(z-t)\omega_{N+1}(z)} = \omega_{N+1}(t) {\sum_{k=0}^{\infty}}' V_k^N(f) T_k(t). \tag{3.6}$$

Since $Q(x, y, c; f) - Q_N(x, y, c; f) = Q(x, y, c; f - p_N)$, using (3.6) in (1.3) and (1.9) gives (3.4). □

From (3.5) and the fact that $|T_k(t)| \leqslant 1$, $|\omega_{N+1}(t)| \leqslant 2$, we have

$$\begin{aligned} |\Omega_k(x, y, c)|/2 &\leqslant \int_x^y |t-c|^\alpha |\log|t-c||\,\mathrm{d}t \\ &\leqslant \int_{-1}^{1} |t-c|^\alpha |\log|t-c||\,\mathrm{d}t =: J_\alpha(c), \quad -1 \leqslant x \leqslant y \leqslant 1, \end{aligned} \tag{3.7}$$

which yields the following Lemma 3.3.

Lemma 3.3. *Let $\phi_\alpha(t)$ be defined by*

$$\phi_\alpha(t) = 2t|t|^\alpha \{\log|t| - 1/(\alpha+1)\}/(\alpha+1), \tag{3.8}$$

namely $\mathrm{d}\phi_\alpha(t)/\mathrm{d}t = 2|t|^\alpha \log|t|$. Assume that $-1 \leqslant x \leqslant c \leqslant y \leqslant 1$. Let $\varphi_\alpha(x, y, c)$ and $\Lambda_\alpha(x, y, c)$ be defined, respectively, by

$$\varphi_\alpha(t) = \begin{cases} -\phi_\alpha(t) & \text{if } |t| \leqslant 1, \\ \phi_\alpha(t) - 2\phi_\alpha(1) & \text{if } t > 1, \\ \phi_\alpha(t) + 2\phi_\alpha(1) & \text{if } t < -1, \end{cases}$$
$$\Lambda_\alpha(x, y, c) = \varphi_\alpha(y-c) - \varphi_\alpha(x-c). \tag{3.9}$$

Then we bound $\Omega_k^N(x, y, c)$ given by (3.5) as follows:

$$|\Omega_k^N(x, y, c)| \leqslant \Lambda_\alpha(x, y, c) \leqslant \Lambda_\alpha(-1, 1, c). \tag{3.10}$$

Following Theorem 3.4 is proven in Section 5.

Theorem 3.4. *Let $\Omega_k^N(x, y, c)$ be defined by* (3.5). *Then $\Omega_k^N(x, y, c)$ is bounded independently of x, y and c, $-1 \leqslant x, y, c \leqslant 1$, by*

$$|\Omega_k^N(x, y, c)| \leqslant \frac{4}{\alpha+1}\left[\frac{1}{\alpha+1} + \max\left\{0, 2^\alpha\left(\log 2 - \frac{1}{\alpha+1}\right)\right\}\right] =: \Gamma_\alpha. \tag{3.11}$$

Suppose that $f(z)$ is a meromorphic function which has M simple poles at the points z_m $(m = 1, 2, \ldots, M)$ outsides $\mathscr{E}_\rho$ with residues $\operatorname{Res} f(z_m)$. Then, performing the contour integral of (3.2) yields

$$V_k^N(f) = -\frac{2}{\pi}\sum_{m=1}^{M} \operatorname{Res} f(z_m)\widetilde{U}_k(z_m)/\omega_{N+1}(z_m), \quad k \geqslant 0. \tag{3.12}$$

Now noting that $T_k(z) = (w^k + w^{-k})/2$ for complex $z = (w + w^{-1})/2 \notin [-1, 1]$ where $|w| > 1$, we have from (1.6) $\omega_{N+1}(z) = \sqrt{z^2-1}(w^N - w^{-N})$, which is combined with (3.3) to yield

$$\widetilde{U}_k(z)/\omega_{N+1}(z) = \pi/\{(z^2-1)(w^N - w^{-N})w^k\}. \tag{3.13}$$

The most dominant term in the right of (3.12) is obtained for the poles z_j for which

$$\left|z_j + \sqrt{z_j^2 - 1}\right| = \min_{1 \leqslant m \leqslant M}\left|z_m + \sqrt{z_m^2-1}\right| \equiv r > 1. \tag{3.14}$$

If we assume that there is only one such z_j, we have $V_k^N(f) \sim V_0^N(f)w_j^{-k}$ for sufficiently large N, where $w_j = z_j + \sqrt{z_j^2-1}$. Here we have used the notation that for $N \geqslant 1$, $a(N) \sim b(N)$ means that $\lim_{N\to\infty} a(N)/b(N) = 1$.

Next, we wish to estimate $|V_0^N(f)|$ in terms of the available coefficients a_k^N of $p_N(t)$. Elliott [4] gives

$$a_k^N = 2(\pi \mathrm{i})^{-1}\oint_{\mathscr{E}_\rho} T_{N-k}(z)f(z)/\omega_{N+1}(z)\,\mathrm{d}z, \quad 0 \leqslant k \leqslant N.$$

Performing the contour integral and comparing the result with (3.12) give the relations $|V_0^N| \sim |a_N^N|r/(r^2-1)$ and $|a_k^N| \sim r|a_{k+1}^N|$ for sufficiently large N. From this fact and (3.4) we get an estimate of the truncation error $E_N(x, y, c; f)$, dependent on or independent of, x, y, and c, for $Q_N(x, y, c; f)$ as follows:

$$E_N(x, y, c; f) = 0.5|a_N^N|\Lambda_\alpha(x, y, c)r/(r-1)^2, \quad -1 \leqslant x \leqslant c \leqslant y \leqslant 1, \tag{3.15}$$

$$E_N(x, y, c; f) = 0.5|a_N^N|\Gamma_\alpha r/(r-1)^2, \quad -1 \leqslant x, y, c \leqslant 1, \tag{3.16}$$

where $\Lambda_\alpha(x, y, c)$ and Γ_α are defined by (3.9) and (3.11), respectively.

Remark. The constant r may be estimated from the asymptotic behavior of $\{a_k^N\}$ [12].

See the numerical example (D) in Section 4 below for the case where r is close to 1.

Incidentally, an automatic quadrature of nonadaptive type is generally constructed from the sequence of approximations $\{Q_N(x, y, c; f)\}$ converging to the integral $Q(x, y, c; f)$ (1.3), until a stopping criterion is satisfied. It is usual and simple way to double the degree N of $p_N(t)$ (1.5) for generating the sequence $\{Q_N(x, y, c; f)\}$ (1.9), see [2,6]. In order to make an automatic quadrature efficient, however, it is advantageous to have more chances of checking the stopping criterion than doubling of N. To this end, as is shown in [13] we may generate the sequence of $\{p_n\}$, by increasing the degree N more slowly as follows:

$$N = 3 \times 2^n, 4 \times 2^n, 5 \times 2^n, \quad n = 1, 2, 3, \ldots, \tag{3.17}$$

and by using the FFT.

Table 1
Comparison in the performance of the present method and QUADPACK

	a	c	Integral value	$\varepsilon_a = 10^{-6}$				10^{-10}			
				Ours		QUADPACK		Ours		QUADPACK	
				N	Error	N	Error	N	Error	N	Error
A	4	0.2	−1.0587127998	17	6E–12	(80)	3E–14	21	9E–15	(80)	3E–14
		1.0	−9.6490968600	17	4E–11	40	5E–14	21	5E–14	40	5E–14
	8	0.2	−0.1090323972	21	1E–10	(80)	1E–15	33	7E–14	(80)	6E–15
		1.0	−8.9486844692	21	2E–10	40	7E–14	33	7E–14	110	6E–14
	16	0.2	−0.02460422656	33	5E–13	(80)	1E–13	33	5E–13	(80)	1E–13
		1.0	−8.1711761827	33	3E–14	80	9E–14	33	3E–14	120	6E–14
B	1	0.2	−21.0961786852	25	8E–11	(80)	7E–13	33	2E–14	(80)	7E–13
		1.0	−5.6876942344	25	8E–11	40	5E–13	33	2E–13	70	9E–14
	1/4	0.2	−212.7691175051	97	1E–8	(120)	9E–12	129	1E–11	(260)	6E–12
		1.0	−11.7691370124	97	8E–12	140	2E–12	129	4E–14	210	5E–13
	1/8	0.2	−423.5776999452	193	5E–8	(190)	4E–12	257	7E–12	(370)	3E–11
		1.0	−12.6751206042	193	2E–12	200	3E–12	257	2E–13	270	5E–13

The numbers of abscissae required to satisfy the tolerances $\varepsilon_a = 10^{-6}$ and 10^{-10} are shown for each problem (A) and (B) with actual errors. The numbers of abscissae in the parentheses are the sum of those required to evaluate two integrals on $[-1, c]$ and $[c, 1]$. The present method gives results for integrals of varied values of c with the common numbers of function evaluations.

4. Numerical examples

Examples in this section were computed in double precision; the machine precision is $2.22\ldots \times 10^{-16}$.

We show here numerical results by the present automatic quadrature scheme for the following definite integrals of algebraic–logarithmic singularities $|t-c|^{\alpha} \log |t-c|$ with $\alpha = -0.7$, in particular

$$\text{(A)} \quad \int_{-1}^{1} \mathrm{e}^{a(t-1)} |t-c|^{\alpha} \log |t-c| \, \mathrm{d}t, \quad a = 4, 8, 16, \quad c = 0.2, 1.0,$$

$$\text{(B)} \quad \int_{-1}^{1} (t^2 + a^2)^{-1} |t-c|^{\alpha} \log |t-c| \, \mathrm{d}t, \quad a = 1, 1/4, 1/8, \quad c = 0.2, 1.0,$$

$$\text{(C)} \quad \int_{0}^{1} \mathrm{e}^{t} \cos(2\pi a t) |t-c|^{\alpha} \log |t-c| \, \mathrm{d}t, \quad a = 8.1, 16.1, 32.1, \quad c = 0.6, 1.0,$$

$$\text{(D)} \quad \int_{0}^{1} \tfrac{1-a^2}{1-2at+a^2} |t-c|^{\alpha} \log |t-c| \, \mathrm{d}t, \quad a = 0.8, 0.9, 0.95, \quad c = 0.6, 1.0.$$

In Tables 1 and 2 we compare the results of the present scheme with those of DQAWS in the subroutine package QUADPACK [20]. The numbers of function evaluations required to satisfy the requested tolerance ε_a are shown in the columns under the title N with actual absolute errors in the columns under the title “error”.

DQAWS is not a routine for approximating indefinite integrals of interior-singular functions. Indeed, DAQWS is a routine for computing definite integrals of functions with algebraic–logarithmic endpoint singularities. To use DQAWS to compute the definite integrals of interior singularities (A) and (B) with $c = 0.2$ and (C)∼(D) with $c = 0.6$, we divide the interval of integration into two parts $[d, c]$ and $[c, 1]$, where $d = -1$ for the problems (A) and (B) and $d = 0$ for the problems (C) and (D). DQAWS is then used to evaluate the integral of endpoint singularity on $[d, c]$ and one on $[c, 1]$, separately. Only for reference, in Tables 1 and 2 we list the results (the numbers of abscissae in the parentheses) of the double use of DAQWS for the integrals of interior singularities with $c = 0.2$ or $c = 0.6$.

The integrand of (D) with a pole at $t = (a + a^{-1})/2$ can be expanded in terms of Chebyshev polynomials $(1 - a^2)/(1 - 2at + a^2) = 2\sum_{k=0}^{\prime\infty} a^k T_k(t)$, $|a| < 1$. If $|a|$ is close to 1, then the Chebyshev expansion converges slowly and the error estimate (3.15) or (3.16) is large since in this case $r = a^{-1}$ is also close to 1. Table 2 shows

Table 2
Comparison in the performance of the present method and QUADPACK

	a	c	Integral value	$\varepsilon_a = 10^{-6}$				10^{-10}			
				Ours		QUADPACK		Ours		QUADPACK	
				N	Error	N	Error	N	Error	N	Error
C	8.1	0.6	−15.7938844062	49	1E–10	(220)	7E–11	65	3E–12	(390)	4E–11
		1.0	−17.7146839939	49	5E–11	210	7E–11	65	9E–13	430	5E–13
	16.1	0.6	11.5613952701	81	2E–10	(480)	1E–11	97	3E–13	(770)	8E–12
		1.0	−15.8096525276	81	6E–12	490	1E–10	97	4E–13	890	1E–12
	32.1	0.6	1.1978745144	161	2E–12	(910)	3E–11	161	2E–12	(1480)	2E–11
		1.0	−13.9868392684	161	2E–12	980	2E–10	161	2E–12	1740	6E–13
D	0.8	0.6	−12.3916250999	65	2E–8	(140)	5E–13	97	4E–12	(170)	1E–13
		1.0	−69.4639879576	65	2E–9	160	3E–13	97	5E–12	240	8E–12
	0.9	0.6	−6.3666333588	161	1E–9	(200)	4E–13	257	3E–13	(230)	2E–13
		1.0	−116.3605746157	161	7E–11	280	8E–12	257	1E–11	380	1E–11
	0.95	0.6	−3.2572791968	321	3E–9	(260)	8E–13	513	2E–13	(290)	2E–13
		1.0	−184.6801824053	321	2E–10	360	1E–11	513	2E–11	560	3E–11

The numbers of abscissae required to satisfy the tolerances $\varepsilon_a = 10^{-6}$ and 10^{-10} are shown for each problem (C) and (D) with actual errors.

that the present method could give approximations satisfying the tolerance to the problem (D) with $a = 0.95$, namely $r = 1.056\ldots$.

It appears that there is no automatic quadrature method to be compared for indefinite integrals of the algebraic–logarithmic singular integrands. We note that the present scheme can efficiently give all the approximations to the integrals (1.3) for a set of the values of c by using a common number of function evaluations once and for all smooth functions.

5. Proof of Theorem 3.4

Since from (3.7) we have $|\Omega_k(x, y, c)| \leqslant 2J_\alpha(c)$, and $J_\alpha(-c) = J_\alpha(c)$, to prove (3.11) it suffices to show

$$\max_{0\leqslant c\leqslant 1} J_\alpha(c) = \frac{2}{\alpha+1}\left[\frac{1}{\alpha+1} + \max\left\{0, 2^\alpha\left(\log 2 - \frac{1}{\alpha+1}\right)\right\}\right]. \tag{5.1}$$

We prove (5.1) for three cases; $-1<\alpha\leqslant 0$, $0<\alpha<1$ and $1\leqslant\alpha$. We begin with the case where $-1<\alpha\leqslant 0$. Let $\psi_\alpha(t)$ be defined by

$$\psi_\alpha(t) = (1-t)^{\alpha+1}\{1/(\alpha+1) - \log(1-t)\}/(\alpha+1), \quad |t|\leqslant 1, \tag{5.2}$$

namely $\mathrm{d}\psi_\alpha(t)\,\mathrm{d}t = (1-t)^\alpha \log(1-t)$ $(|t|<1)$. Then we from (3.7) have

$$J_\alpha(c) = 2\psi_\alpha(0) + \psi_\alpha(c) - \psi_\alpha(-c), \quad 0\leqslant c\leqslant 1. \tag{5.3}$$

Since

$$\mathrm{d}J_\alpha(c)/\mathrm{d}c = (1-c)^\alpha\log(1-c) + (1+c)^\alpha\log(1+c), \quad 0\leqslant c\leqslant 1, \tag{5.4}$$

and $\mathrm{d}J_\alpha(c)/\mathrm{d}c\leqslant 0$ for $-1<\alpha\leqslant 0$, we have

$$\max_{0\leqslant c\leqslant 1} J_\alpha(c) = J_\alpha(0) = 2/(\alpha+1)^2, \quad -1<\alpha\leqslant 0.$$

Now we consider the case where $0<\alpha$. Since

$$J_\alpha(1) = 2/(\alpha+1)^2 + 2^{\alpha+1}\{\log 2 - 1/(\alpha+1)\}/(\alpha+1),$$

to verify (5.1), it is enough to show that for $0 < \alpha$,

$$\max_{0\leqslant c\leqslant 1} J_\alpha(c) = \max\{J_\alpha(0), J_\alpha(1)\}. \tag{5.5}$$

When $\alpha\geqslant 1$ we can easily verify (5.5) since $J_\alpha(c)$ is convex in [0, 1]. In fact

$$\mathrm{d}^2 J_\alpha(c)/\mathrm{d}c^2 = \alpha\{(1+c)^{\alpha-1}\log(1+c) - (1-c)^{\alpha-1}\log(1-c)\} + (1+c)^{\alpha-1} - (1-c)^{\alpha-1} \geqslant 0.$$

On the other hand, when $0 < \alpha < 1$ to prove (5.5) we need the following Lemma 5.1.

Lemma 5.1. *Let $g(x)$ be a function continuous on* [0, 1] *which has a Maclaurin expansion*

$$g(x) = \sum_{k=0}^{\infty} a_k x^k, \quad 0\leqslant x < 1,$$

with the convergence radius of unity. Assume that there exists a positive integer n such that $a_k \leqslant 0$ if $1\leqslant k\leqslant n$, otherwise $a_k \geqslant 0$. Then we have

$$\max_{0\leqslant x\leqslant 1} g(x) = \max\{g(0), g(1)\}. \tag{5.6}$$

Proof. It is trivial that (5.6) holds either if $g'(x)\leqslant 0$ $(0\leqslant x < 1)$ or if $g'(x)\geqslant 0$ $(0\leqslant x < 1)$. Otherwise, from the mean value theorem there exists $\xi \in (0, 1)$ such that $g'(\xi) = 0$. Let $g'(\xi)$ be written by

$$0 = g'(\xi) = \sum_{k=0}^{n-1} b_k \xi^k + \sum_{k=n}^{\infty} b_k \xi^k, \tag{5.7}$$

where we set $b_k = (k+1)a_{k+1}$. From the assumption it follows that $b_k \leqslant 0$ $(0\leqslant k < n)$ and $b_k \geqslant 0$ $(n\leqslant k)$. It remains to show that $g(x)$ monotonically decreases in $(0, \xi)$ and increases in $(\xi, 1)$. To this end we show $g'(x)\leqslant 0$ $(0 < x < \xi)$ and $g'(x)\geqslant 0$ $(\xi < x < 1)$. It is easy to see that $g'(x) = \sum_{k=0}^{\infty} b_k x^k \leqslant 0$ $(0 < x < \xi)$ since

$$\sum_{k=n}^{\infty} b_k x^k \leqslant \left(\frac{x}{\xi}\right)^n \sum_{k=n}^{\infty} b_k \xi^k \leqslant \left(\frac{x}{\xi}\right)^{n-1} \sum_{k=n}^{\infty} b_k \xi^k = -\left(\frac{x}{\xi}\right)^{n-1} \sum_{k=0}^{n-1} b_k \xi^k \leqslant -\sum_{k=0}^{n-1} b_k x^k,$$

where we have used (5.7) and the fact that $(x/\xi)^k \leqslant (x/\xi)^n$ if $n\leqslant k$. Similarly we have $g'(x)\geqslant 0$ $(\xi < x < 1)$ since

$$\begin{aligned}\sum_{k=n}^{\infty} b_k x^k &\geqslant \left(\frac{x}{\xi}\right)^n \sum_{k=n}^{\infty} b_k \xi^k \geqslant \left(\frac{x}{\xi}\right)^{n-1} \sum_{k=n}^{\infty} b_k \xi^k \\ &= -\left(\frac{x}{\xi}\right)^{n-1} \sum_{k=0}^{n-1} b_k \xi^k \geqslant -\sum_{k=0}^{n-1} b_k x^k. \qquad \square\end{aligned}$$

Now we use Lemma 5.1 to prove (5.5). Let $\psi_\alpha(t)$ defined by (5.2) be expanded in the form

$$\psi_\alpha(t) = \sum_{k=0}^{\infty} d_k t^k / k!, \quad |t| < 1. \tag{5.8}$$

Then from (5.3) we have

$$J_\alpha(c) = 2d_0 + 2\sum_{k=0}^{\infty} d_{2k+1} c^{2k+1}/(2k+1)!. \tag{5.9}$$

From (5.8) and (5.9) we see that it is enough to show that $\psi_\alpha(t)$ satisfies the assumption in Lemma 5.1 to verify (5.5) for $0<\alpha<1$. Simple manipulations of (5.2) and (5.8) reveal that $\psi_\alpha^{(k)}(0)=d_k$ and

$$\psi_\alpha^{(k)}(t)=(1-t)^{\alpha+1-k}\{d_k-\gamma_k\log(1-t)\},\quad 0\leqslant t<1,$$

where the coefficients d_k and γ_k are given, respectively, by

$$d_k=(k-\alpha-2)d_{k-1}+\gamma_{k-1},\quad \gamma_k=(k-\alpha-2)\gamma_{k-1},\quad k\geqslant 1, \tag{5.10}$$

and $d_0=1/(\alpha+1)^2$, $\gamma_0=1/(\alpha+1)$. Particularly, $\gamma_1=-1$, $\gamma_2=\alpha$, $d_1=0$ and $d_2=\gamma_1=-1$. Since $\psi_\alpha^{(2)}(0)=d_2<0$ and $\psi_\alpha^{(1)}(0)=\psi_\alpha^{(1)}(1)=0$, it is impossible that $\psi_\alpha^{(2)}(t)<0$ for all $t\in[0,1)$. Therefore, it follows that there exists $n>2$ such that $d_k\leqslant 0$ for $1\leqslant k<n$ and $d_n>0$, where $\psi_\alpha^{(2)}(t)=\sum_{k=0}^{\infty}d_{k+2}t^k/k!$. The recurrence relations (5.10) shows

$$\gamma_k=-(0-\alpha)(1-\alpha)\cdots(k-2-\alpha)>0,\quad k\geqslant 2.$$

With this relation and (5.10) the induction on k shows that $d_k>0$ for $k>n$. Thus, we have verified that $\psi_\alpha(t)$ satisfies the assumption in Lemma 5.1.

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